

Topological Hierarchy Insulators and Topological Fractal Insulators

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Topological insulators are new states of quantum matter with metallic edge/surface states. In this paper, we pointed out that there exists a new type of particle-hole symmetry-protected topological insulator - topological hierarchy insulator (THI), a composite topological state of a (parent) topological insulator and its defect-induced topological mid-gap states. A particular type of THI is topological fractal insulator, that is a THI with self-similar topological structure. In the end, we discuss the possible experimental realizations of THIs.

Recently, a new research topic focuses on searching for topologically nontrivial phases protected by symmetries. Topological band insulator (TBI) provides an example of symmetry-protected topological states, in which there exist metallic edge/surface states[1, 2]. According to the characterization of "ten-fold way" of different symmetries[3], there are two types of TBIs in two dimensions: Z-type TBI with integer quantum Hall effect[4] and Z_2 -type TBI with quantum spin-Hall effect[1, 5–8]. Then, people found that with extending the topological classification of band structures to include considering crystal point group symmetries, there exists new type of TBI - topological crystalline insulators[9]. Those additional symmetries lead to a non-trivial topology of bulk wave functions and gapless edge/surface states.

For TBIs, owing to the "holographic feature", their nontrivial topological properties can be detected by probing topological defects. For example, in two dimensional (2D) Z-type TBIs, π -flux traps mid-gap zero energy states (zero modes) [10–12]. For this topological state with a superlattice of π -fluxes, due to the polygon rule (Each fermion gains an accumulated phase shift $|\phi| = (n - 2)\pi/2$ encircling around a smallest n-polygon rule [13]), the defect-induced mid-gap states can be regarded as an emergent "TBI" with nontrivial topological properties, including the nonzero Chern number and the gapless edge states[14].

In this paper we point out that a new kind of topological insulator - *topological hierarchy insulator* may exist, in which the topological properties are protected by translational and (generalized) particle-hole symmetry. In this system, the non-topological lattice defect - *vacancy* traps zero mode[15]. For the system with vacancy-superlattice, the ground state becomes topological hierarchy insulator (THI). To show the nontrivial topological properties of THI, we take the Haldane model on square lattice and that on honeycomb lattice as examples. We found that the vacancy-superlattice could induce topological mid-gap states and the low energy physics of the localized modes become that of an emergent "TBI" on the parent TBI. In particular, the so-called *topologi-*

cal fractal insulator appears as a special THI with *self-similar* topological structure.

The Haldane model on square lattice: Our starting point is the (spinless) Haldane model on square lattice[16, 17], of which the Hamiltonian is

$$\begin{aligned} \hat{H}_{\text{parent}} = & -t \sum_{i \in A} \left(\hat{c}_{i+\hat{x}}^\dagger \hat{c}_i + i \hat{c}_{i+\hat{y}}^\dagger \hat{c}_i + h.c. \right) \\ & + t \sum_{i \in B} \left(\hat{c}_{i+\hat{x}}^\dagger \hat{c}_i - i \hat{c}_{i+\hat{y}}^\dagger \hat{c}_i + h.c. \right) \\ & - t' \sum_{i \in A} \left(\hat{c}_{i+\hat{x}+\hat{y}}^\dagger \hat{c}_i + \hat{c}_{i+\hat{x}-\hat{y}}^\dagger \hat{c}_i + h.c. \right) \\ & + t' \sum_{i \in B} \left(\hat{c}_{i+\hat{x}+\hat{y}}^\dagger \hat{c}_i + \hat{c}_{i+\hat{x}-\hat{y}}^\dagger \hat{c}_i + h.c. \right) \quad (1) \end{aligned}$$

where \hat{c}_i is the annihilation operator of the fermions at the site i . A and B label the sublattices. t and t' are the nearest neighbor (NN) and the next nearest neighbor (NNN) hoppings, respectively. For the Hamiltonian in Eq.(1), there exists π -flux in each square plaquette and $\frac{\pi}{2}$ -flux in each triangular lattice. In this paper we set the lattice spacing a to be unit.

The Haldane model on square lattice is a TBI with quantum anomalous Hall (QAH) effect. There is a finite energy gap near points $\mathbf{k}_1 = (0, 0)$ and $\mathbf{k}_2 = (\pi, 0)$ which is $\Delta_f = 8t'$. The Chern number C_{parent} of (parent) Haldane model is 1 and the quantized Hall conductivity is $\frac{e^2}{h}$.

In particular, we point out that the Hamiltonian in Eq.(1) has the particle-hole (PH) symmetry. Under PH transformation, we have $\hat{H}_{\text{parent}} = -\mathcal{P}^\dagger \hat{H}_{\text{parent}} \mathcal{P}$ where $\mathcal{P} = \mathcal{R} \cdot \mathcal{K}$ is the PH transformation operator[15, 18]. Here, \mathcal{R} is an operator that leads to $\hat{c}_i \leftrightarrow (-1)^i \hat{c}_i^\dagger$ and \mathcal{K} is the complex conjugate operator. As a result, each energy level with positive energy E is paired with an energy level with negative energy $-E$. Because the Hamiltonian in Eq.(1) is on a bipartite lattice, the quantum levels of the system with a single vacancy become an odd integer number. As a result, there must exist an unpaired electronic state when we remove a lattice-site to create a vacancy. Due to PH symmetry, the corresponding unpaired electronic state must have exactly zero energy[15]. We denote the wave-function of the zero mode by $\psi_0(r_i - R)$ where R is the position of the vacancy. The quantum

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states of the fermionic zero mode around a vacancy can be formally described in terms of the fermion Fock states $\{|0\rangle, |1\rangle\}$. Here, $|0\rangle, |1\rangle$ denote the empty state, and the occupied state, respectively.

Topological hierarchy insulator: We next study the Haldane model with vacancy-superlattice (VSL). When there are two vacancies nearby, the inter-vacancy quantum tunneling effect occurs and the fermionic zero modes on two vacancies couple. The lattice constant of the VSL is denoted by L , which is the distance between two vacancies nearby. When the vacancies locate at the different sublattices, the energy splitting ΔE is finite (L/a is an odd number); when the vacancies locate at the same sublattice, the energy splitting vanishes, $\Delta E = 0$ (L/a is an even number). For the case of $\xi < L$, we can consider each vacancy as an isolated "atom" with localized electronic states and use the effective tight-binding model to describe these quantum states induced by the VSL. Now, we superpose the localized states to obtain the sets of Wannier wave functions $\psi_0(r_i - R)$. In general, the effective tight-binding model of the localized states induced by the VSL becomes

$$\begin{aligned} \hat{H}_{1-VL} = & - \sum_{\langle R, R' \rangle} T_{RR'} \hat{d}_R^\dagger \hat{d}_{R'} - \sum_{\langle\langle R, R' \rangle\rangle} T'_{RR'} \hat{d}_R^\dagger \hat{d}_{R'} \quad (2) \\ & - \sum_{\langle\langle\langle R, R' \rangle\rangle\rangle} T''_{RR'} \hat{d}_R^\dagger \hat{d}_{R'} + \dots, \end{aligned}$$

where \hat{d}_R is the fermionic annihilation operator of a localized state on a vacancy R . $T_{RR'}$ ($T'_{RR'}$, $T''_{RR'}$) is the hopping parameter between NN (NNN, NNNN) sites R and R' and is determined by the energy splitting $\Delta E_{RR'}$, $|T_{RR'}| = |\Delta E|$ ($|T'_{RR'}| = |\Delta E'|$, $|T''_{RR'}| = |\Delta E''|$). In general, due to $|T'_{RR'}| \ll |T_{RR'}|$, $|T''_{RR'}|$, we only consider the NN hopping term and NNN hopping term. Because the parent Hamiltonian in Eq.(1) has PH symmetry, the effective tight-binding model of the localized states induced by the VSL \hat{H}_{1-VL} in Eq.(2) also has PH symmetry, $\hat{H}_{1-VL} = -\mathcal{P}^\dagger \hat{H}_{1-VL} \mathcal{P}$.

Because the energy splitting $\Delta E_{RR'}$ only determines the particle's hopping amplitude $|T_{RR'}|$, we need to settle down the phase of $T_{RR'}$. In particular, to preserve PH symmetry, the total phase around a plaquette with four vacancies can be either π or 0. An approach is to count the total flux number inside the plaquette. For the mid-gap states induced by VSL, every four vacancies form an $L \times L$ square, of which the total flux number is just $L^2/2$ and the total phase around a plaquette is πL^2 . After considering the compact condition, we have $0/\pi$ -flux inside each plaquette if L^2 is an even/odd number. In addition, we also use a numerical approach to check above prediction of the flux number inside the plaquette.

Based on the Haldane model, we study the properties of a PH symmetry-protected TBI with VSL and introduce the concept of *topological hierarchy insulator*. To make it clear, we take the Haldane model with *square-VSL* as an example, of which the lattice constant L is $3a$. See the illustration in Fig.1.(a). From above discussion,

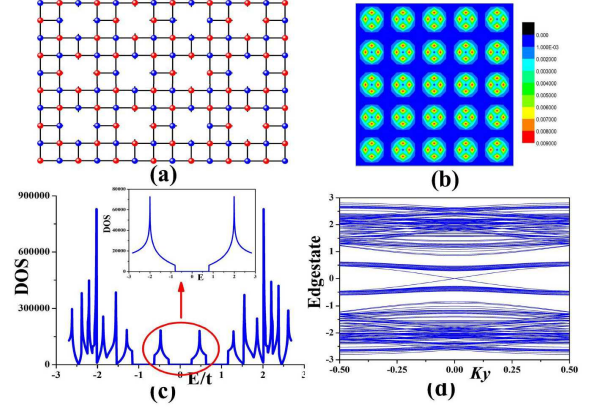


FIG. 1: (Color online) (a) The illustration of square-VSLs on square lattice; (b) The particle distribution of zero modes around vacancies; (c) The DOS of the Haldane model with square-VSL for $L = 3a$: the mid-gap states are induced by the square-VSL. The inset shows the DOS of the parent Haldane model; (d) The edge states of mid-gap states. The parameter is $t'/t = 0.2$.

there exists π -flux in each square plaquette of VSL and $\pi/2$ -flux in each triangular VSL. Fig.1.(b) is the configuration of zero modes around vacancies. From Fig.1.(b), one can see that quantum states induced by VSL can be regarded as a new generation of lattice model, of which the vacancies play the role of the "atoms".

As a result, we obtain an effective Hamiltonian to describe the vacancy-induced mid-gap states, that reads

$$\begin{aligned} \hat{H}_{1-VL} = & -T \sum_{R \in \bar{A}} (\hat{d}_{R+L\hat{x}}^\dagger \hat{d}_R + i\hat{d}_{R+L\hat{y}}^\dagger \hat{d}_R + h.c.) \quad (3) \\ & + T \sum_{R \in \bar{B}} (\hat{d}_{R+L\hat{x}}^\dagger \hat{d}_R - i\hat{d}_{R+L\hat{y}}^\dagger \hat{d}_R + h.c.) \\ & + T' \sum_{i \in \bar{A}} (\hat{d}_{R+L\hat{x}+L\hat{y}}^\dagger \hat{d}_R + \hat{d}_{R+L\hat{x}-L\hat{y}}^\dagger \hat{d}_R + h.c.) \\ & - T' \sum_{i \in \bar{B}} (\hat{d}_{R+L\hat{x}+L\hat{y}}^\dagger \hat{d}_R + \hat{d}_{R+L\hat{x}-L\hat{y}}^\dagger \hat{d}_R + h.c.) \end{aligned}$$

where T, T' are effective NN and NNN hopping parameters, respectively. \bar{A} and \bar{B} label the sublattices of VSL. By comparing Eq.(1) and Eq.(3), one can see the corresponding relationship, $\hat{c}_i \longleftrightarrow \hat{d}_R$, $t \longleftrightarrow T$, $t' \longleftrightarrow -T'$. For the defect-induced quantum states, the energy spectrum and DOS are obviously similar to those of the parent Hamiltonian in Eq.(1).

In Fig.1.(c) we show the DOS of the Haldane model with square-VSL for $t'/t = 0.2$ and $L = 3a$. In Fig.1.(c), the mid-gap (MG) energy bands appear and the DOS of the MG states is really similar to that of the parent TBI (the inset in Fig.1.(c)). We obtain the hopping parameters by fitting the DOS of the defect-induced quantum states as $T = 0.22t$ and $T' = 0.07t$.

In addition, we will show the MG states induced by VSL have similar topological properties to those of par-

ent TBI. By the numerical approach, we found that the Chern number of the MG states is $C_{1-\text{VL}} = -1$ which opposites to that of parent TBI as $C_{1-\text{VL}} = -C_{\text{parent}}$. To characterize the THI, we define the filling factor, $\nu = N_f/N$ where N is the total number of lattice sites and N_f is the number of fermions. The composite system is an insulator at filling factor $\nu = \frac{1}{2}$ or $\nu = \frac{1}{2}(1 - \frac{a^2}{L^2})$. At half filling (or $\nu = \frac{1}{2}$), the total Chern number of the system is zero due to $C_{\text{total}} = C_{\text{parent}} + C_{1-\text{VL}}$; at filling factor $\frac{1}{2}(1 - \frac{a^2}{L^2})$, the total Chern number of the system is 1 due to $C_{\text{total}} = C_{\text{parent}}$.

To illustrate the topological properties of the Haldane model with square-VSL, we then study its edge states. On one hand, at the filling factor $\frac{1}{2}(1 - \frac{a^2}{L^2})$, the system becomes a TBI with Chern number 1. As a result, when the system has periodic boundary condition along y -direction but open boundary condition along x -direction, there exist the gapless edge states. On the other hand, we consider the half filling case, of which the system has zero Chern number. However, the system still has nontrivial topological properties. When the parent topological insulator has periodic boundary condition along both x -direction and y -direction, while the VSL has periodic boundary condition along y -direction but open boundary condition along x -direction, there may exist gapless edge states. See the numerical results in Fig.1.(d) for the case of $L = 3a$. We can see that there indeed exist gapless edge states on the boundaries of VSL.

In general, the Haldane model with a square-VSL of odd number L^2 has nontrivial topological properties and is different from traditional TBIs. As a result, we call this type of PH symmetry-protected TBI with topological MG states to be *topological hierarchy insulator*. In other words, the point of view THI is given by the following equation

$$\begin{aligned} \text{THI} &= \text{PH symmetry-protected TBI} \\ &+ L \times L\text{-square-VSL} \\ &= \text{Parent TBI} + \text{topological MG states.} \end{aligned} \quad (4)$$

Topological fractal insulator: We then study a particular type of THI - topological fractal insulator (TFI), that is a THI with infinite generations of self-similar $L \times L$ -square-VSLs. See the illustration in Fig.2.(a).

To construct a TFI, firstly we consider a THI with self-similar MG states. Because we can tune T'/T (or $\Delta E'/\Delta E$) by changing the NNN hopping t' of the parent TBI or the VSL constant L , the MG states can be self-similar to the parents states for the case of $T/T' = t/t'$. After numerical calculations, we obtain the self-similar condition in Fig.2.(b). See the dots in Fig.2.(b). According to the phase diagram of Fig.2.(b), smaller/bigger t/t' leads to bigger/smaller T/T' . Now, under the self-similar condition $T/T' = t/t'$, the effective Hamiltonian that describes the MG states becomes $\hat{H}_{1-\text{VL}} = \alpha \hat{H}_{\text{parent}}^*$ where $\alpha = T/t$ ($\alpha < 1$) is an energy-scaling ratio.

Next, we regard the vacancy-induced MG states as a parent TBI and consider an additional VSL on it. So,

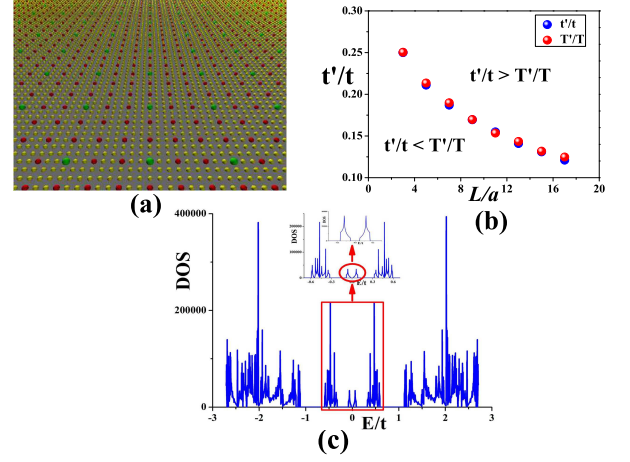


FIG. 2: (Color online) (a) An illustration of the VSLs for TFI; (b) The self-similar condition; (c) The DOS of TFI. The parameter is $t'/t = 0.2$. The insets show the DOSs of the mid-gap states.

using the recursive relation, we can see that there exist additional MG states inside the energy gap of first generation MG states (we call it generation-1 MG states). Consequently, we get a new generation of topological MG states (we call such MG states in the energy gap of MG states as generation-2 MG states). Using the same method, we can construct a THI with n -generation MG states and eventually a THI with infinite generations of self-similar MG states that is just a TFI. Then, under the self-similar condition $T/T' = t/t'$, the effective Hamiltonian of the generation- n MG states is given by

$$\hat{H}_{n-\text{VL}} = \begin{cases} \alpha^n \hat{H}_{\text{parent}}, & n \text{ is an even number,} \\ \alpha^n \hat{H}_{\text{parent}}^*, & n \text{ is an odd number.} \end{cases} \quad (5)$$

From the DOS in Fig.2.(c), we can see that the DOS of the MG states is always self-similar.

In addition, we discuss the Chern number of the TFI. The TFI is an insulator at filling factor $\nu = \frac{1}{2}(1 - \frac{a^{2m}}{L^{2m}})$ where m is an integer number, $m \geq 1$. The Chern number of generation- m MG states is known to be $C_{m-\text{VL}} = (-1)^m$. As a result, when the filling factor is $\nu = \frac{1}{2}(1 - \frac{a^{2m}}{L^{2m}})$, the total Chern number of the system is

$$C_{\text{total}} = C_{\text{parent}} + \sum_{n=1}^{m-1} C_{n-\text{VL}} = [1 + (-1)^{m-1}]/2. \quad (6)$$

For example, when the filling factor is $\frac{1}{2}(1 - \frac{a^6}{L^6})$ ($m = 3$), the total Chern number of the system is 1 due to $C_{\text{total}} = C_{\text{parent}} + C_{1-\text{VL}} + C_{2-\text{VL}}$.

It is known that a self-similar object looks "roughly" the same on different scales and fractal is a particularly self-similar object that exhibits a repeating pattern displaying at every scale. Topological fractal insulator provides a unique example of topological matters with

self-similarity, in which the topological properties always look the same on different energy scales (α^{2n}) or different length scales (L^{2n}).

Topological hierarchy insulators on honeycomb lattice: We finally study the THI based on the Haldane model on honeycomb lattice, of which the Hamiltonian is given by

$$\hat{H}_{\text{parent}} = -t \sum_{\langle i,j \rangle} \hat{c}_i^\dagger \hat{c}_j - t' \sum_{\langle\langle i,j \rangle\rangle} e^{i\phi_{ij}} \hat{c}_i^\dagger \hat{c}_j - \mu \sum_i \hat{c}_i^\dagger \hat{c}_i \quad (7)$$

where \hat{c}_i represents the fermion annihilation operator at site i . t and t' are the nearest neighbor (NN) and the next nearest neighbor (NNN) hoppings, respectively. $e^{i\phi_{ij}}$ is a complex phase along the NNN link, and we set the direction of the positive phase is clockwise ($|\phi_{ij}| = \frac{\pi}{2}$). μ is the chemical potential. The Haldane model on honeycomb lattice is also a Chern insulator with nonzero Chern number, $C_{\text{parent}} = 1$.

Since the Haldane model of Eq.(7) also satisfies the PH symmetry [15], $\hat{H}_{\text{parent}} = -\mathcal{P}^\dagger \hat{H}_{\text{parent}} \mathcal{P}$, a vacancy induces a fermionic zero mode. In the followings, we focus on the Haldane model with honeycomb-VSL shown in Fig.3.(a), of which the distance between two vacancies with shortest distance L is $5a$. The particle density distribution of fermionic zero modes induced by VSL is shown in Fig.3.(b).

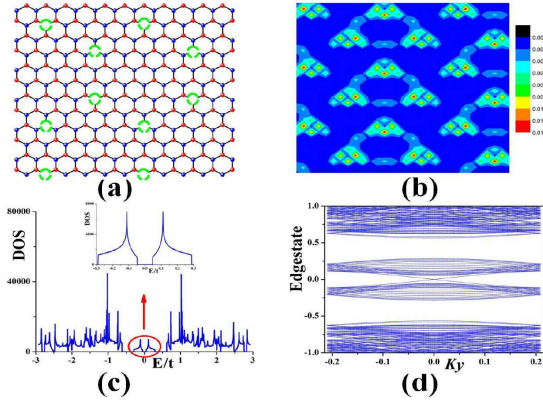


FIG. 3: (Color online) (a) The illustration of honeycomb-VSL on honeycomb lattice. The distance between two vacancies is $5a$; (b) The particle distribution of zero modes around vacancies; (c) The DOS of the Haldane model with honeycomb-VSL. The insets show the DOSs of the mid-gap states; (d) The edge states of mid-gap states. The parameter is $t'/t = 0.1$.

Using similar approach, we derive an effective Hamiltonian to describe the MG states

$$\hat{H}_{\text{I-VL}} = -T \sum_{\langle I,J \rangle} \hat{d}_I^\dagger \hat{d}_J - T' \sum_{\langle\langle I,J \rangle\rangle} e^{-i\phi_{IJ}} \hat{d}_I^\dagger \hat{d}_J - \mu \sum_I \hat{d}_I^\dagger \hat{d}_I \quad (8)$$

where T, T' are effective NN and NNN hopping parameters, respectively. I, J denote the positions of a vacancies. By comparing Eq.(7) and Eq.(8), one can see the

corresponding relationship to be $\hat{c}_i \longleftrightarrow \hat{d}_I$, $t \longleftrightarrow T$, $t' \longleftrightarrow T'$, $\phi_{ij} \rightarrow -\phi_{IJ}$.

The DOS of the THI on honeycomb lattice is shown in Fig.3.(c). There exist MG states induced by honeycomb-VSL, of which the DOS is also similar to that of the parent Hamiltonian in Eq.(7). Next, we calculate the Chern number of the THI on honeycomb lattice and find that the Chern number of the MG states $C_{\text{I-VL}}$ is -1 which also opposites to the parent TBI, $C_{\text{parent}} = -C_{\text{I-VL}}$. The THI is an insulator at filling factor $\nu = \frac{1}{2}$ or $\nu = \frac{24}{50}$. At half filling (or $\nu = \frac{1}{2}$), the total Chern number of the system is zero; at filling factor $\nu = \frac{24}{50}$, the total Chern number of the system is 1. In addition, we study the edge states of the MG states. See the numerical results in Fig.3.(d). For a THI with n -generation MG states, the total Chern number of the system at filling factor $\nu = \frac{1}{2}(1 - \frac{2^n}{L^{2n}})$ is $[1 + (-1)^{n-1}]/2$.

Discussion and conclusion: In this paper, based on the Haldane model on square lattice and that on honeycomb lattice, we studied the Chern insulators with VSL and found the vacancy-induced MG states have nontrivial topological properties. Then, we discover new types of TBI - THIs and TFIs. All these topological insulators are protected by particle-hole symmetry. In particular, TFIs provide a unique example of topological matters with self-similarity, in which the topological properties always look the same on different energy scales. As a result, these exotic properties of THIs and TFIs will deepen our understanding of symmetry-protected topological states. In the future, similar topological states (THIs or TFIs) can be explored on other lattices (for example, the triangular lattice or kagome lattice).

Finally, we address the relevant experimental realizations of the THI. In condensed matter physics, it is difficult to realize the Haldane model. However, the Kane-Mele (KM) model can be regarded as two copies of the Haldane model such that the spin up electron and the spin down electron exhibit opposite Chern number[1]. Because the KM model also has PH symmetry, THI can be designed based on it. Ref. [19] proposed that the KM model can be realized in a silicene-based material with a honeycomb lattice. A possible vacancy in silicene is a missing Si-atom that can be regarded as a vacancy in the KM model. For the silicene with periodic pattern of missing Si-atoms, the THI may be possible realized. On the other hand, experimental realizations of quantum many-body systems in optical lattices have led to a chance to simulate a variety of topological states. Recently, in Ref.[20], the (spinless) Haldane model on honeycomb optical lattice has been simulated in the cold atoms. Because the VSL on optical lattice may be achieved by holographic method, THI may be realized on optical lattice by using timely cold-atom technology.

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